Graphs with Diameter n - eMinimizing the Spectral Radius

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Abstract

The spectral radius $\rho(G)$ of a graph G is the largest eigenvalue of its adjacency matrix A(G). For a fixed integer $e \geq 1$, let $G_{n,n-e}^{min}$ be a graph with minimal spectral radius among all connected graphs on n vertices with diameter n-e. Let $P_{n_1,n_2,\dots,n_t,p}^{m_1,m_2,\dots,m_t}$ be a tree obtained from a path of p vertices $(0 \sim 1 \sim 2 \sim \cdots \sim (p-1))$ by linking one pendant path P_{n_i} at m_i for each $i \in \{1,2,\dots,t\}$. For e=1,2,3,4,5, $G_{n,n-e}^{min}$ were determined in the literature. Cioabă-van Dam-Koolen-Lee [2] conjectured for fixed $e \geq 6$, $G_{n,n-e}^{min}$ is in the family $\mathcal{P}_{n,e} = \{P_{2,1,\dots,1,2,n-e+1}^{2,m_2,\dots,m_{e-4},n-e-2} \mid 2 < m_2 < \dots < m_{e-4} < n-e-2\}$. For e=6,7, they conjectured $G_{n,n-6}^{min} = P_{2,1,2,n-5}^{2,\lceil \frac{D-1}{2}\rceil,D-2}$ and $G_{n,n-7}^{min} = P_{2,1,1,2,n-6}^{2,\lceil \frac{D+1}{2}\rceil,D-2}$. In this paper, we settle their conjectures positively. Note that any tree in $\mathcal{P}_{n,e}$ is uniquely determined by its internal path lengths. For any e-4 non-negative integers k_1,k_2,\dots,k_{e-4} , let $T_{(k_1,k_2,\dots,k_{e-4})} = P_{2,1,\dots,1,2,n-e+1}^{2,m_2,\dots,m_{e-4},n-e-2}$ with $k_i = m_{i+1} - m_i - 1$, for $1 \leq i \leq e-4$. (Here we assume $m_1 = 2$ and $m_{e-3} = n-e-2$.)

Let $s = \frac{\sum_{i=1}^{e-4} k_i + 2}{e-4}$. For any integer $e \ge 6$ and sufficiently large n, we proved that $G_{n,n-e}^{min}$ must be one of the trees $T_{(k_1,k_2,\dots,k_{e-4})}$ with the parameters satisfying $\lfloor s \rfloor - 1 \le k_j \le \lfloor s \rfloor \le k_i \le \lceil s \rceil + 1$ for j = 1, e-4 and $i = 2,\dots,e-5$. Moreover, $0 \le k_i - k_j \le 2$ for $2 \le i \le e-5$, j = 1, e-4; and $|k_i - k_j| \le 1$ for $2 \le i, j \le e-5$. These results are best possible as shown by cases e = 6, 7, 8, where $G_{n,n-e}^{min}$ are completely determined here. Moreover, if n-6 is divisible by e-4 and n is sufficiently large, then $G_{n,e}^{min} = T_{(k-1,k,k,\dots,k,k,k-1)}$ where $k = \frac{n-6}{e-4} - 2$.

1 Introduction

Let G = (V, E) be a simple connected graph, and A(G) be the adjacency matrix of G. The characteristic polynomial of G is defined by $\phi_G(\lambda) = \det(\lambda I - A(G))$. The spectral radius, denoted by $\rho(G)$, is the largest root of ϕ_G . The problem of determining graphs with small spectral radius can be traced back to Hoffman and Smith [10, 7, 8]. They completely determined all connected graphs G with $\rho(G) \leq 2$. The connected graphs with $\rho(G) < 2$ are precisely simple Dynkin Diagrams A_n , D_n , E_6 , E_7 , and E_8 . The connected graphs with $\rho(G) = 2$ are exactly those simple extended Dynkin Diagrams \tilde{A}_n , \tilde{D}_n , \tilde{E}_6 , \tilde{E}_7 , and \tilde{E}_8 . Cvetković et al. [4] gave a nearly complete description of all graphs G with $0 \leq 2$ with $0 \leq 2$. Their description was completed by Brouwer and Neumaier [1]. Those graphs are some special trees with at most two

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vertices of degree 3. Wang et al. [12] studied some graphs with spectral radius close to $\frac{3}{2}\sqrt{2}$. Woo and Neumaier [13] determined the structures of graphs G with $\sqrt{2+\sqrt{5}} \le \rho(G) \le \frac{3}{2}\sqrt{2}$; if G has maximum degree at least 4, then G is a dagger (i.e., a path is attached to a leaf of a star S_4); if G is a tree with maximum degree at most 3, then G is an $open\ quipus$ (i.e., the vertices of degree 3 lies on a path); else G is a $closed\ quipus$ (i.e., a unicyclic graph with maximum degree at most 3 satisfies that the vertices of degree 3 lies on a cycle).

Van Dam and Kooij [3] used the following notation to denote an open quipus. Let $P_{n_1,n_2,\dots n_t,p}^{m_1,m_2,\dots m_t,p}$ be a tree obtained from a path on p vertices $(0 \sim 1 \sim 2 \sim \cdots \sim (p-1))$ by linking one pendant path P_{n_i} at m_i for $i=1,2,\dots,t$ (see Figure 1.) The path $0 \sim 1 \sim 2 \sim \cdots \sim (p-1)$ is called main path. For $i=1,\dots,t-1$, let $P^{(i)}$ be the i-th internal path $(m_i \sim m_i+1 \sim \cdots \sim m_{i+1})$ and $k_i=m_{i+1}-m_i-1$ be the number of internal vertices on $P^{(i)}$. In general, an internal path in G is a path $v_0 \sim v_1 \sim \cdots \sim v_s$ such that $d(v_0) > 2$, $d(v_s) > 2$, and $d(v_i) = 2$, whenever 0 < i < s. An internal path is closed if $v_0 = v_s$.

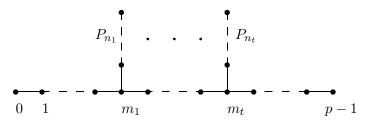


Figure 1: $P_{n_1,n_2,...,n_t,p}^{m_1,m_2,...,m_t}$

Recently van Dam and Kooij [3] asked an interesting question "which connected graph of order n with a given diameter D has minimal spectral radius?". Here the diameter of a connected graph is the maximum distance among all pairs of its vertices. They [3] solved this problem explicitly for graphs with diameter $D \in \{1, 2, \lfloor n/2 \rfloor, n-3, n-2, n-1\}$. The cases D=1 and D=n-1 are trivial. A minimizer graph, denoted by $G_{n,D}^{min}$, is a graph that has the minimal spectral radius among all the graphs of order n and diameter D. They proved that $G_{n,2}^{min}$ is either a star or a Moore graph; $G_{n,\lfloor n/2 \rfloor}^{min}$ is the cycle C_n ; $G_{n,n-2}^{min}$ is the tree $P_{1,n-1}^1$; $G_{n,n-3}^{min}$ is the tree $P_{1,1,n-2}^{1,n-4}$. They conjectured $G_{n,n-e}^{min} = P_{\lfloor \frac{e-1}{2} \rfloor, \lceil \frac{e-1}{2} \rceil, n-e+1}^{\lfloor \frac{e-1}{2} \rfloor, \lceil \frac{e-1}{2} \rceil, n-e+1}$ for any constant $e \geq 1$ and $e \geq 1$ and

This conjecture is proved for e=4 by Yuan et al. [5] and for e=5 by Cioabă et al. [2]. However, it is disproved for e=6 by [11] and any $e\geq 6$ by [2] when n large enough. Cioabă-van Dam-Koolen-Lee [2] proved the following theorem.

Theorem 5.2 of [2]: For $e \geq 6$, $\rho(G_{n,n-e}^{min}) \rightarrow \sqrt{2+\sqrt{5}}$ as $n \rightarrow \infty$. Moreover $G_{n,n-e}^{min}$ is contained in one of the following three families of graphs

$$\mathcal{P}_{n,e} = \left\{ P_{2,1,\dots,1,2,n-e+1}^{2,m_2,\dots,m_{e-4},n-e-2} \mid 2 < m_2 < \dots < m_{e-4} < n-e-2 \right\},$$

$$\mathcal{P}'_{n,e} = \left\{ P_{2,1,\dots,1,1,n-e+1}^{2,m_2,\dots,m_{e-3},n-e-1} \mid 2 < m_2 < \dots < m_{e-3} < n-e-1 \right\},$$

$$\mathcal{P}''_{n,e} = \left\{ P_{1,1,\dots,1,1,n-e+1}^{1,m_2,\dots,m_{e-2},n-e-1} \mid 1 < m_2 < \dots < m_{e-2} < n-e-1 \right\}.$$

Cioabă et al. [2] made three conjectures.

Conjecture 1 ([2], 5.3) For fixed $e \geq 5$, a minimizer graph with n vertices and diameter D = n - e is in the family $\mathcal{P}_{n,e}$, for n large enough.

Conjecture 2 ([2], 5.4) The graph $P_{2,1,2,n-5}^{2,\lceil \frac{D-1}{2}\rceil,D-2}$ is the unique minimizer graph with n vertices and diameter D=n-6, for n large enough.

Conjecture 3 ([2], 5.5) The graph $P_{2,1,1,2,n-6}^{2,\lfloor\frac{D+2}{3}\rfloor,D-\lfloor\frac{D+2}{3}\rfloor,D-2}$ is the unique minimizer graph with n vertices and diameter D=n-7, for n large enough. ¹

In this paper, we settle these three conjectures positively.

Note that graphs in each family can be determined by the lengths of internal paths (see Figure 2). The parameters k_i 's and m_i 's are related as follows. In the first family $\mathcal{P}_{n,e}$, $T_{(k_1,k_2,\dots,k_{e-4})} = P_{2,1,\dots,2,n-e+1}^{2,m_2,\dots,m_{e-4},n-e-2}$ if $k_i = m_{i+1} - m_i - 1$ for $1 \le i \le e-4$, where $m_1 = 2$ and $m_{e-3} = n-e-2$. In the second family $\mathcal{P}'_{n,e}$, $T'_{(k_1,k_2,\dots,k_{e-3})} = P_{2,1,\dots,1,n-e+1}^{2,m_2,\dots,m_{e-3},n-e-1}$ if $k_i = m_{i+1} - m_i - 1$ for $1 \le i \le e-3$, where $m_1 = 2$ and $m_{e-2} = n-e-1$. In the third family $\mathcal{P}''_{n,e}$, $T''_{(k_1,k_2,\dots,k_{e-2})} = P_{1,1,\dots,1,n-e+1}^{1,m_2,\dots,m_{e-2},n-e-1}$ if $k_i = m_{i+1} - m_i - 1$ for $1 \le i \le e-2$, where $m_1 = 1$ and $m_{e-1} = n-e-1$. In all three cases, the summation of all k_i 's is always equal to n-2e.

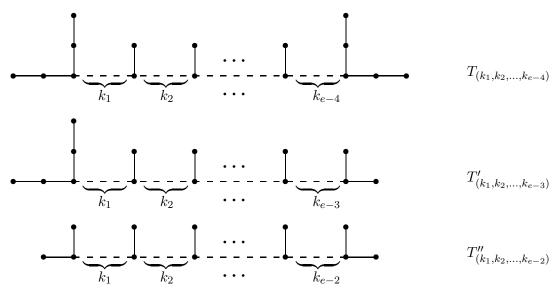


Figure 2: The three families of graphs: $\mathcal{P}_{n,e}$, $\mathcal{P}'_{n,e}$, $\mathcal{P}''_{n,e}$.

We have the following theorem.

Theorem 1.1 For any $e \ge 6$ and sufficiently large n, $G_{n,n-e}^{min}$ must be a tree $T_{(k_1,k_2,...,k_{e-4})}$ in $\mathcal{P}_{n,e}$ satisfying

- 1. $\lfloor s \rfloor 1 \le k_j \le \lfloor s \rfloor \le k_i \le \lceil s \rceil + 1$ for $2 \le i \le e 5$ and j = 1, e 4, where $s = \frac{n-6}{e-4} 2$,
- 2. $0 \le k_i k_j \le 2$ for $2 \le i \le e 5$ and j = 1, e 4,
- 3. $|k_i k_j| \le 1$ for $2 \le i, j \le e 5$.

In particular, if n-6 is divisible by e-4, then $G_{n,n-e}^{min}=T_{(s-1,s,\ldots,s,s-1)}$.

Here we completely determine the $G_{n,n-e}^{min}$ for e=6,7,8 and settle the conjectures 2 and 3 positively.

¹Conjecture 5.5 of [2] contains a typo: "... $P_{2,1,1,2,n-6}^{2,\lfloor \frac{D-2}{3}\rfloor,D-\lfloor \frac{D-2}{3}\rfloor,D-2}$...".

Theorem 1.2 For e = 6 and n large enough, $G_{n,n-e}^{min}$ is unique up to a graph isomorphism.

- 1. If n = 2k + 12, then $G_{n,n-6}^{min} = T_{(k,k)}$.
- 2. If n = 2k + 13, then $G_{n,n-6}^{min} = T_{(k,k+1)}$.

Theorem 1.3 For e = 7 and n large enough, $G_{n,n-e}^{min}$ is unique up to a graph isomorphism.

- 1. If n = 3k + 14, then $G_{n,n-7}^{min} = T_{(k,k,k)}$.
- 2. If n = 3k + 15, then $G_{n,n-7}^{min} = T_{(k,k+1,k)}$.
- 3. If n = 3k + 16, then $G_{n,n-7}^{min} = T_{(k,k+2,k)}$.

Theorem 1.4 For e = 8 and n large enough, $G_{n,n-e}^{min}$ is determined up to a graph isomorphism as follows.

- 1. If n = 3k + 16, then $G_{n,n-8}^{min} = T_{(k,k,k,k)}$, $T_{(k,k,k+1,k-1)}$, or $T_{(k-1,k+1,k+1,k-1)}$; all three trees have the same spectral radius.
- 2. If n = 3k + 17, then $G_{n,n-8}^{min} = T_{(k,k+1,k,k)}$.
- 3. If n = 3k + 18, then $G_{n,n-8}^{min} = T_{(k,k+1,k+1,k)}$.
- 4. If n = 3k + 19, then $G_{n,n-8}^{min} = T_{(k,k+1,k+2,k)}$.

For e = 6, Theorem 1.2 is an easy corollary of Theorem 1.1. Theorem 1.3 and Theorem 1.4 show that the bounds on k_i 's in Theorem 1.1 are best possible.

The remaining of the paper is organized as follows. In section 2, we prove some useful lemmas. The proof of Theorem 1.1 is presented in section 3 and the proofs of Theorem 1.3 and 1.4 are given in section 4.

2 Basic notations and Lemmas

2.1 Preliminary results

For any vertex v in a graph G, let N(v) be the neighborhood of v. Let G - v be the remaining graph of G after deleting the vertex v (and all edges incident to v). Similarly, G - u - v is the remaining graph of G after deleting two vertices u, v. Here are some basic facts found in literature [6, 7, 9, 11], which will be used later.

Lemma 2.1 [6] Suppose that G is a connected graph. If v is not in any cycle of G, then $\phi_G = \lambda \phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v}$. If e = uv is a cut edge of G, then $\phi_G = \phi_{G-e} - \phi_{G-u-v}$.

Lemma 2.2 [6] Let G_1 and G_2 be two graphs, then the following statements hold.

- 1. If G_2 is a proper subgraph of G_1 , then $\rho(G_1) > \rho(G_2)$.
- 2. If G_2 is a spanning proper subgraph of G_1 , then $\rho(G_1) > \rho(G_2)$ and $\phi_{G_2}(\lambda) > \phi_{G_1}(\lambda)$ for all $\lambda \geq \rho(G_1)$.
- 3. If $\phi_{G_2}(\lambda) > \phi_{G_1}(\lambda)$ for all $\lambda \geq \rho(G_1)$, then $\rho(G_2) < \rho(G_1)$.
- 4. If $\phi_{G_1}(\rho(G_2)) < 0$, then $\rho(G_1) > \rho(G_2)$.

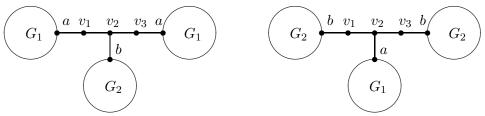


Figure 3: The graphs H_1 and H_2

Lemma 2.3 [11] Let G_1 and G_2 be two (possibly empty) graphs with $a \in V(G_1)$ and $b \in V(G_2)$, and let H_1 and H_2 be two graphs shown in Figure 3. Then $\rho(H_1) = \rho(H_2)$.

Lemma 2.4 [7] Let uv be an edge of a connected graph G of order n, and denote by $G_{u,v}$ the graph obtained from G by subdividing the edge uv once, i.e., adding a new vertex w and edges wu, wv in G - uv. Then the following two properties hold.

- 1. If uv does not belong to an internal path of G and $G \neq C_n$, then $\rho(G_{u,v}) > \rho(G)$.
- 2. If uv belongs to an internal path of G and $G \neq P_{1,1,n}^{1,n-2}$, then $\rho(G_{u,v}) < \rho(G)$.

Theorem 2.1 (Cauchy Interlace Theorem (see p.183, [9])) Let A be a Hermitian matrix of order n, and let B be a principal submatrix of A of order n-1. If $\lambda_n \leq \lambda_{n-1} \leq \cdots \leq \lambda_1$ lists the eigenvalues of A and $\mu_{n-1} \leq \mu_{n-2} \leq \cdots \leq \mu_1$ the eigenvalues of B, then

$$\lambda_n \le \mu_{n-1} \le \lambda_{n-1} \le \dots \le \lambda_2 \le \mu_1 \le \lambda_1.$$

Applying Cauchy Interlace Theorem to the adjacency matrices of graphs, we have the following corollary.

Corollary 2.1 Suppose G is a connected graph. Let $\lambda_2(G)$ be the second largest eigenvalue of G. For any vertex v, we have

$$\lambda_2(G) < \rho(G - v) < \rho(G).$$

2.2 Our approach

A rooted graph (G, v) is a graph G together with a designated vertex v as a root. For i = 1, 2, 3 and a given rooted graph (H, v'), we get a new rooted graph (G_i, v) from H by attaching a path P_i to v' and changing the root from v' to v as shown by Figure 4.

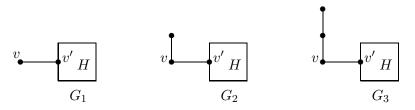


Figure 4: For i = 1, 2, 3, three graphs (G_i, v) are constructed from (H, v').

Note that any tree in the three families $\mathcal{P}_{n,e}$, $\mathcal{P}''_{n,e}$, $\mathcal{P}''_{n,e}$ can be built up from a single vertex through a sequence of three operations above. Applying Lemma 2.1, we observe that the pair $(\phi_{G_i}, \phi_{G_i-v})$ linearly depends on $(\phi_H, \phi_{H-v'})$ with coefficients in $\mathbb{Z}[\lambda]$. We can choose proper base to diagonalize the operation from (H, v') to (G_1, v) .

Let λ_0 be the constant $\sqrt{2+\sqrt{5}}=2.058\cdots$. In this paper, we consider only the range $\lambda \geq \lambda_0$. Let x_1 and x_2 be two roots of the equation $x^2-\lambda x+1=0$. We have

$$x_1 = \frac{\lambda - \sqrt{\lambda^2 - 4}}{2}, \quad x_2 = \frac{\lambda + \sqrt{\lambda^2 - 4}}{2}$$

and

$$x_1 + x_2 = \lambda, \quad x_1 x_2 = 1.$$
 (1)

For any vertex v in a graph G, we define two functions (of λ) $p_{(G,v)}$ and $q_{(G,v)}$ satisfying

$$\phi_G = p_{(G,v)} + q_{(G,v)},$$

$$\phi_{G-v} = x_2 p_{(G,v)} + x_1 q_{(G,v)}.$$

This definition can be written in the following matrix form:

$$\begin{pmatrix} \phi_G \\ \phi_{G-v} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix} \begin{pmatrix} p_{(G,v)} \\ q_{(G,v)} \end{pmatrix}. \tag{2}$$

Using Equation (1), we can solve $p_{(G,v)}$ and $q_{(G,v)}$ and get

$$\begin{pmatrix} p_{(G,v)} \\ q_{(G,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1 & 1 \\ x_2 & -1 \end{pmatrix} \begin{pmatrix} \phi_G \\ \phi_{G-v} \end{pmatrix}. \tag{3}$$

For example, let v be the center of the odd path P_{2k+1} . We have

$$\begin{pmatrix} p_{(P_1,v)} \\ q_{(P_1,v)} \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} -x_1^2 \\ x_2^2 \end{pmatrix}, \tag{4}$$

$$\begin{pmatrix} p_{(P_3,v)} \\ q_{(P_3,v)} \end{pmatrix} = \lambda \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}, \tag{5}$$

$$\begin{pmatrix} p_{(P_5,v)} \\ q_{(P_5,v)} \end{pmatrix} = \frac{\lambda^2 - 1}{x_2 - x_1} \begin{pmatrix} (\lambda - x_1^3) x_1 \\ (x_2^3 - \lambda) x_2 \end{pmatrix}. \tag{6}$$

We have the following lemma.

Lemma 2.5 For any tree G and any vertex v, we have

$$\lim_{\lambda \to +\infty} q_{(G,v)}(\lambda) = +\infty. \tag{7}$$

Proof From Lemma 2.1, we have

$$\phi_G = \lambda \phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v}.$$

By Equation (3), we get

$$q_{(G,v)} = \frac{1}{x_2 - x_1} (x_2 \phi_G - \phi_{G-v})$$

$$= \frac{1}{x_2 - x_1} \left(x_2 \left(\lambda \phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v} \right) - \phi_{G-v} \right)$$

$$= \frac{1}{x_2 - x_1} \left((\lambda x_2 - 1) \phi_{G-v} - x_2 \sum_{w \in N(v)} \phi_{G-w-v} \right)$$

$$= \frac{x_2}{x_2 - x_1} \left(x_2 \phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v} \right).$$

Note that ϕ_{G-v} is a polynomial of degree n-1 with highest coefficient 1 while ϕ_{G-w-v} is a polynomial of degree n-2 with highest coefficient 1. Since $x_2 > 1 > x_1$, we have $x_2\phi_{G-v} - \sum_{w \in N(v)} \phi_{G-w-v}$ goes to infinity as λ approaches infinity.

Lemma 2.6 Let G_1, G_2, G_3 be the graphs shown in Figure 4. Then the following equations hold.

1.
$$\begin{pmatrix} p_{(G_1,v)} \\ q_{(G_1,v)} \end{pmatrix} = \begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}.$$

$$2. \left(\begin{array}{c} p_{(G_2,v)} \\ q_{(G_2,v)} \end{array}\right) = \frac{1}{x_2 - x_1} \left(\begin{array}{cc} \lambda - x_1^3 & x_1 \\ -x_2 & x_2^3 - \lambda \end{array}\right) \left(\begin{array}{c} p_{(H,v')} \\ q_{(H,v')} \end{array}\right).$$

$$3. \ \left(\begin{array}{c} p_{(G_3,v)} \\ q_{(G_3,v)} \end{array} \right) = \frac{1}{x_2-x_1} \left(\begin{array}{cc} -x_1^4 + \lambda^2 - 1 & \lambda x_1 \\ -\lambda x_2 & x_2^4 - \lambda^2 + 1 \end{array} \right) \left(\begin{array}{c} p_{(H,v')} \\ q_{(H,v')} \end{array} \right).$$

Proof By Lemma 2.1, we have

$$\begin{pmatrix} \phi_{G_1} \\ \phi_{G_1-v} \end{pmatrix} = \begin{pmatrix} \lambda & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \phi_H \\ \phi_{H-v'} \end{pmatrix}.$$

Combining it with equations (2) (3), we get

$$\begin{pmatrix} p_{(G_1,v)} \\ q_{(G_1,v)} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix}^{-1} \begin{pmatrix} \lambda & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ x_2 & x_1 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}$$
$$= \frac{1}{x_2 - x_1} \begin{pmatrix} 2 - \lambda x_1 & x_1^2 - \lambda x_1 + 1 \\ -x_2^2 + \lambda x_2 - 1 & \lambda x_2 - 2 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}$$
$$= \begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix} \begin{pmatrix} p_{(H,v')} \\ q_{(H,v')} \end{pmatrix}.$$

The proofs of items 2 and 3 are similar as that of item 1.

We denote the three matrices by A, B, and C. Namely,

$$A = \left(\begin{array}{cc} x_1 & 0 \\ 0 & x_2 \end{array} \right), B = \frac{1}{x_2 - x_1} \left(\begin{array}{cc} \lambda - x_1^3 & x_1 \\ -x_2 & x_2^3 - \lambda \end{array} \right), C = \frac{1}{x_2 - x_1} \left(\begin{array}{cc} -x_1^4 + \lambda^2 - 1 & \lambda x_1 \\ -\lambda x_2 & x_2^4 - \lambda^2 + 1 \end{array} \right).$$

The diagonal elements of B are very useful parameters. To simplify our notations later, we define two parameters d_1 and d_2 as follows:

$$d_1 = \lambda - x_1^3, \tag{8}$$

$$d_2 = x_2^3 - \lambda. (9)$$

Note that $d_2 = 0$ if $\lambda = \lambda_0$. The equation (6) can be written as

$$\begin{pmatrix} p_{(P_5,v)} \\ q_{(P_5,v)} \end{pmatrix} = \frac{\lambda^2 - 1}{x_2 - x_1} \begin{pmatrix} d_1 x_1 \\ d_2 x_2 \end{pmatrix}. \tag{10}$$

From the definitions of d_1 and d_2 , we can derive the following identity

$$d_1 x_2 - d_2 x_1 = 2. (11)$$

Given two rooted graphs (H_1, v_1) and (H_2, v_2) , we define some new graphs. Denote by $(H_1, v_1) \cdot P_i$, the graph consisting of the graph H_1 and a path P_i linking one of its ends at the vertex v_1 . Similarly denote by $(H_1, v_1) \cdot P_i \cdot (H_2, v_2)$ the graph consisting of graphs H_1, H_2 and a path P_i linking the two ends at v_1, v_2 respectively.

$$H_1 v_1 \qquad \qquad u \qquad \qquad v_2 H_2$$

Figure 5: The graph $(H_1, v_1) \cdot P_1 \cdot (H_2, v_2)$

Lemma 2.7
$$\phi_{(H_1,v_1)\cdot P_1\cdot (H_2,v_2)}(\lambda) = (x_2-x_1)(q_{(H_1,v_1)}q_{(H_2,v_2)}-p_{(H_1,v_1)}p_{(H_2,v_2)}).$$

Proof By Lemmas 2.1 and 2.6, we have

$$\begin{split} \phi_{(H_{1},v_{1})\cdot P_{1}\cdot (H_{2},v_{2})}(\lambda) &= \lambda \phi_{H_{1}}\phi_{H_{2}} - \phi_{H_{1}-v_{1}}\phi_{H_{2}} - \phi_{H_{2}-v_{2}}\phi_{H_{1}} \\ &= (x_{1}+x_{2})(p_{(H_{1},v_{1})}+q_{(H_{1},v_{1})})(p_{(H_{2},v_{2})}+q_{(H_{2},v_{2})}) - (p_{(H_{1},v_{1})}x_{2}+q_{(H_{1},v_{1})}x_{1}) \\ &\quad (p_{(H_{2},v_{2})}+q_{(H_{2},v_{2})}) - (p_{(H_{1},v_{1})}+q_{(H_{1},v_{1})})(p_{(H_{2},v_{2})}x_{2}+q_{(H_{2},v_{2})}x_{1}) \\ &= (p_{(H_{2},v_{2})}+q_{(H_{2},v_{2})})(p_{(H_{1},v_{1})}x_{1}+q_{(H_{1},v_{1})}x_{2}) - (p_{(H_{1},v_{1})}+q_{(H_{1},v_{1})})(p_{(H_{2},v_{2})}x_{2}+q_{(H_{2},v_{2})}x_{1}) \\ &= p_{(H_{2},v_{2})}p_{(H_{1},v_{1})}x_{1}+q_{(H_{2},v_{2})}q_{(H_{1},v_{1})}x_{2}-p_{(H_{2},v_{2})}p_{(H_{1},v_{1})}x_{2}-q_{(H_{2},v_{2})}q_{(H_{1},v_{1})}x_{1} \\ &= (x_{2}-x_{1})(q_{(H_{1},v_{1})}q_{(H_{2},v_{2})}-p_{(H_{1},v_{1})}p_{(H_{2},v_{2})}). \end{split}$$

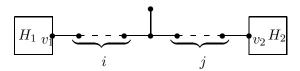


Figure 6: The graph $G_{i,j}$

Lemma 2.8 Let $G_{i,j}$ be the graph shown in Figure 6 where i, j are the numbers of included vertices. Then

$$\phi_{G_{i,j}} - \phi_{G_{i+1,j-1}} = (x_1 - x_2) \left(p_{(H_1,v_1)} q_{(H_2,v_2)} x_2^{j-i-1} - q_{(H_1,v_1)} p_{(H_2,v_2)} x_1^{j-i-1} \right).$$

Proof By lemma 2.1, we have

$$\begin{array}{rcl} \phi_{G_{i,j}} & = & \lambda \phi_{(H_1,v_1) \cdot P_{i+j+1} \cdot (H_2,v_2)} - \phi_{(H_1,v_1) \cdot P_i} \phi_{(H_2,v_2) \cdot P_j}, \\ \phi_{G_{i+1,j-1}} & = & \lambda \phi_{(H_1,v_1) \cdot P_{i+j+1} \cdot (H_2,v_2)} - \phi_{(H_1,v_1) \cdot P_{i+1}} \phi_{(H_2,v_2) \cdot P_{j-1}}. \end{array}$$

Thus, we get

$$\begin{split} \phi_{G_{i,j}} - \phi_{G_{i+1,j-1}} &= \phi_{(H_1,v_1) \cdot P_{i+1}} \phi_{(H_2,v_2) \cdot P_{j-1}} - \phi_{(H_1,v_1) \cdot P_i} \phi_{(H_2,v_2) \cdot P_j} \\ &= \left(p_{(H_1,v_1)} x_1^{i+1} + q_{(H_1,v_1)} x_2^{i+1} \right) \left(p_{(H_2,v_2)} x_1^{j-1} + q_{(H_2,v_2)} x_2^{j-1} \right) \\ &- \left(p_{(H_1,v_1)} x_1^i + q_{(H_1,v_1)} x_2^i \right) \left(p_{(H_2,v_2)} x_1^j + q_{(H_2,v_2)} x_2^j \right) \\ &= p_{(H_1,v_1)} q_{(H_2,v_2)} \left(x_1^{i+1} x_2^{j-1} - x_1^i x_2^j \right) + q_{(H_1,v_1)} p_{(H_2,v_2)} \left(x_1^{j-1} x_2^{i+1} - x_1^j x_2^i \right) \\ &= x_1^i x_2^i \left[p_{(H_1,v_1)} q_{(H_2,v_2)} (x_1 x_2^{j-i-1} - x_2^{j-i}) + q_{(H_1,v_1)} p_{(H_2,v_2)} (x_1^{j-i-1} x_2 - x_1^{j-i}) \right] \\ &= (x_1 - x_2) \left(p_{(H_1,v_1)} q_{(H_2,v_2)} x_2^{j-i-1} - q_{(H_1,v_1)} p_{(H_2,v_2)} x_1^{j-i-1} \right). \end{split}$$

The proof is completed.

Lemma 2.9 Suppose G_1 and G_2 are two connected graphs satisfying $G_1 - u_1 = G_2 - u_2$ for some vertices $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$. If $\phi_{G_2}(\rho(G_1)) > 0$, then $\rho(G_1) > \rho(G_2)$.

Proof Let $G = G_1 - u_1 = G_2 - u_2$. By Corollary 2.1, we have

$$\rho(G_i) > \rho(G) \ge \lambda_2(G_i) \quad \text{for } i = 1, 2.$$

Here $\lambda_2(G_i)$ is the second largest eigenvalue of G_i . We have $\rho(G_1) > \lambda_2(G_2)$. Since $\rho(G_2)$ is a simple root and $\lim_{\lambda \to \infty} \phi_{G_2}(\lambda) = +\infty$, we have

$$\phi_{G_2}(\lambda) < 0$$
 for $\lambda \in (\lambda_2(G_2), \rho(G_2))$.

Since $\phi_{G_2}(\rho(G_1)) > 0$ and $\rho(G_1) > \lambda_2(G_2)$, we must have $\rho(G_1) > \rho(G_2)$.

2.3 A special tree $T_{(k-1,k,\ldots,k,k-1)}$

The tree $T_{(k-1,k,...,k,k-1)}$ ($\in \mathcal{P}_{n,e}$) plays an important role in this paper. We have the following lemma.

Lemma 2.10 The spectral radius of the tree $T_{(k-1,k,...,k,k-1)}$ is the unique root ρ_k of the equation $d_2 = \frac{2x_1^k}{1-x_1^{k+1}}$ in the interval $\left(\sqrt{2+\sqrt{5}},\infty\right)$.

Remark 1: The following equations are equivalent to one another.

$$d_2 = \frac{2x_1^k}{1 - x_1^{k+1}},$$

$$d_2x_2^k - d_1x_1^k = 2,$$

$$d_2 = d_1x_1^{k-1},$$

$$d_2x_2^{\frac{k-1}{2}} = d_1x_1^{\frac{k-1}{2}},$$

$$d_2 = 2x_1^k + d_1x_1^{2k}.$$

If "=" is replaced by "≥", then these inequalities are still equivalent to each other. These equivalences can be proved by equation (11). The details are omitted.

Remark 2: For any $k \ge 4$, we have $\rho_k \le \rho_4 < \frac{3}{2}\sqrt{2}$. For any $e \ge 6$ and $n \ge (k+2)(e-4)+6$, we can obtain a tree T on n vertices and diameter n-e by subdividing some edges on internal paths of $T_{(k-1,k,\ldots,k,k-1)}$. By Lemma 2.4, we have

$$\rho(T) \le \rho(T_{(k-1,k,\dots,k,k-1)}) = \rho_k < \frac{3}{2}\sqrt{2}.$$

In particular, for $e \ge 6$ and $n \ge (k+2)(e-4)+6 = |T_{(k-1,k,\dots,k,k-1)}|$, we have $\rho(G_{n,n-e}^{min}) < \frac{3}{2}\sqrt{2}$. In the set of graphs with spectral radius at most $\sqrt{2+\sqrt{5}}$ (see [1]), there is no graph with diameter n-e for $e \ge 6$. Thus, $\rho(G_{n,n-e}^{min}) \ge \sqrt{2+\sqrt{5}}$.

Proof of Lemma 2.10. Let $G = T_{(k-1,k,\dots,k,k-1)}$ and v be the leftmost vertex. Note that G can be built up from a single vertex with a series of three operations as specified in Lemma 2.6.

We have

$$\phi_{G} = (1,1) \begin{pmatrix} p_{(T_{(k-1,k,\dots,k,k-1)},v)} \\ q_{(T_{(k-1,k,\dots,k,k-1)},v)} \end{pmatrix}$$

$$= (1,1)A^{2}CA^{k-1}BA^{k}...BA^{k-1}CA \begin{pmatrix} 1 & 1 \\ x_{2} & x_{1} \end{pmatrix}^{-1} \begin{pmatrix} \lambda \\ 1 \end{pmatrix}$$

$$= \frac{(\lambda^{2}-1)^{2}}{x_{2}-x_{1}}(-d_{1},d_{2})A^{k-1}BA^{k}...BA^{k-1} \begin{pmatrix} d_{1}x_{1} \\ d_{2}x_{2} \end{pmatrix}$$

$$= \frac{(\lambda^{2}-1)^{2}}{x_{2}-x_{1}}(-d_{1},d_{2})A^{k-1}BA^{k}...BA^{k} \begin{pmatrix} d_{1} \\ d_{2} \end{pmatrix}.$$

Let $l = \frac{k-1}{2}$; l does not have to be an integer. Define $A^l = \begin{pmatrix} x_1^l & 0 \\ 0 & x_2^l \end{pmatrix}$. We can write ϕ_G as

$$\phi_G = \frac{(\lambda^2 - 1)^2}{x_2 - x_1} (-d_1 x_1^l, d_2 x_2^l) (A^l B A^{l+1})^{r-1} \begin{pmatrix} d_1 x_1^l \\ d_2 x_2^l \end{pmatrix}. \tag{12}$$

It is easy to calculate

$$A^{l}BA^{l+1} = \frac{1}{x_2 - x_1} \begin{pmatrix} d_1 x_1^k & 1\\ -1 & d_2 x_2^k \end{pmatrix}. \tag{13}$$

Now we prove that ρ_k is a root of ϕ_G . At $\lambda = \rho_k$, we have $d_1 x_1^l = d_2 x_2^l$ and $d_1 x_1^k + 1 = d_2 x_2^k - 1$. Thus

$$(A^{l}BA^{l+1}) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{x_2 - x_1} \begin{pmatrix} d_1 x_1^k & 1 \\ -1 & d_2 x_2^k \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= \frac{d_1 x_1^k + 1}{x_2 - x_1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

We have

$$\phi_G(\rho_k) = \frac{(\lambda^2 - 1)^2}{x_2 - x_1} (-d_1 x_1^l, d_2 x_2^l) (A^l B A^{l+1})^{r-1} \begin{pmatrix} d_1 x_1^l \\ d_2 x_2^l \end{pmatrix}$$

$$= \frac{(\lambda^2 - 1)^2}{(x_2 - x_1)^r} (d_1 x_1^k + 1)^{r-1} d_1^2 x_1^{k-1} (-1, 1) \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= 0.$$

It remains to prove $\phi_G(\lambda) > 0$ for any $\lambda > \rho_k$. When $\lambda > \rho_k$, we have $d_2x_2^k - 1 > d_1x_1^k + 1$ (and $d_2x_2^l > d_1x_1^l$). It is easy to check A^lBA^{l+1} maps the region $\{(z_1, z_2) \colon z_2 \geq z_1 > 0\}$ to $\{(z_1, z_2) \colon z_2 > z_1 > 0\}$. By induction on r, $(A^lBA^{l+1})^{r-1}$ maps the region $\{(z_1, z_2) \colon z_2 \geq z_1 > 0\}$ to $\{(z_1, z_2) \colon z_2 > z_1 > 0\}$. Let

$$\left(\begin{array}{c} z_1\\ z_2 \end{array}\right) = (A^l B A^{l+1})^{r-1} \left(\begin{array}{c} d_1 x_1^l\\ d_2 x_2^l \end{array}\right).$$

Since $d_2x_2^l > d_1x_1^l > 0$, we have $z_2 > z_1 > 0$. From equation (12), we get

$$\phi_{G} = \frac{(\lambda^{2} - 1)^{2}}{x_{2} - x_{1}} (-d_{1}x_{1}^{l}, d_{2}x_{2}^{l}) (A^{l}BA^{l+1})^{r-1} \begin{pmatrix} d_{1}x_{1}^{l} \\ d_{2}x_{2}^{l} \end{pmatrix}$$

$$= \frac{(\lambda^{2} - 1)^{2}}{x_{2} - x_{1}} (-d_{1}x_{1}^{l}, d_{2}x_{2}^{l}) \begin{pmatrix} z_{1} \\ z_{2} \end{pmatrix}$$

$$= \frac{(\lambda^{2} - 1)^{2}}{x_{2} - x_{1}} (d_{2}x_{2}^{l}z_{2} - d_{1}x_{1}^{l}z_{1})$$

$$> 0.$$

The proof of the Lemma is finished.

2.4 Limit points of some graphs

Using the tools developed in the previous section, we can compute the limit point of the spectral radius of some graphs.

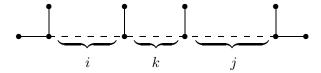


Figure 7: The graphs $T''_{(i,k,j)}$

Lemma 2.11 Let $T''_{(i,k,j)}$ be the tree shown in Figure 7 and ρ''_k be the unique root of $d_2 = x_1^k$ in the interval $\left(\sqrt{2+\sqrt{5}},+\infty\right)$. Then $\lim_{i,j\to\infty}\rho(T''_{(i,k,j)})=\rho''_k$.

Proof By Lemma 2.4, we have

$$\rho(T''_{(i,k,i)}) \ge \rho(T''_{(i,k,j)} \ge T''_{(j,k,j)} \quad \text{if } i \le j.$$

It suffices to show $\lim_{l\to\infty} \rho(T''_{(l,k,l)}) = \rho''_k$. Let v be the leftmost vertex of $T''_{(l,k,l)}$. A simple calculation shows

$$\begin{split} & \phi_{T_{(l,k,l)}''} \\ &= \quad (1,1) \left(\begin{array}{c} p_{(T_{(l,k,l)}',v)} \\ q_{(T_{(l,k,l)}',v)} \end{array} \right) \\ &= \quad (1,1)ABA^lBA^kBA^lB \left(\begin{array}{c} 1 & 1 \\ x_2 & x_1 \end{array} \right)^{-1} \left(\begin{array}{c} \lambda \\ 1 \end{array} \right) \\ &= \quad \frac{x_2^{2l-k+1}(d_2x_2+x_1^2)^2}{(x_2-x_1)^5} \left[((d_2x_2^k)^2-1)-2x_1^{2l-k+3}(d_1x_1^k+d_2x_2^k)-x_1^{2(2l-k+3)}((d_1x_1^k)^2-1) \right]. \end{split}$$

As l goes to infinity, $\lim_{l\to\infty} \rho(T''_{(l,k,l)})$ is the largest root of $(d_2x_2^k)^2 - 1 = 0$; namely $d_2 = x_1^k$. The proof is completed.

We have the following Corollary from Lemma 2.11.

Corollary 2.2 Let $T''_{(k,i)}$ be the tree shown in Figure 8. We have $\lim_{i\to\infty} \rho(T''_{(k,i)}) = \rho''_{2k+3}$.

Proof By Lemma 2.3, we have
$$\rho(T''_{(k,i)}) = \rho(T''_{(i,2k+3,i)})$$
. Thus $\lim_{i \to \infty} \rho(T''_{(k,i)}) = \lim_{i \to \infty} \rho(T''_{(i,2k+3,i)}) = \rho''_{2k+3}$.

Lemma 2.12 Let $T'_{(k,j)}$ be the tree shown in Figure 9 and ρ'_k be the unique root of $d_2 = d_1^{\frac{1}{2}} x_1^{k+\frac{1}{2}}$ in the interval $\left(\sqrt{2+\sqrt{5}},+\infty\right)$. Then $\lim_{j\to\infty}\rho(T'_{(k,j)})=\rho'_k$.



Figure 8: The graph T''(k,i)

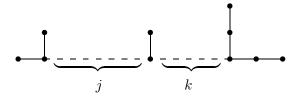


Figure 9: The graph T'(k,j)

Proof Similarly, we have

$$\phi_{T'_{(k,j)}} = (1,1) \begin{pmatrix} p_{(T'_{(k,j)},v)} \\ q_{(T'_{(k,j)},v)} \end{pmatrix}
= (1,1)ABA^{j}BA^{k}CA \begin{pmatrix} 1 & 1 \\ x_{2} & x_{1} \end{pmatrix}^{-1} \begin{pmatrix} \lambda \\ 1 \end{pmatrix}
= \frac{x_{2}^{j+k+1}(\lambda^{2}-1)(d_{2}x_{2}+x_{1}^{3})}{(x_{2}-x_{1})^{3}} \left(d_{2}^{2}-d_{1}x_{1}^{2k+1}-d_{2}x_{1}^{2j+3}-d_{1}^{2}x_{1}^{2j+2k+4}\right)$$

As j goes to infinity, $\lim_{J\to\infty} \rho(T'_{(k,j)})$ is the largest root of $d_2^2 = d_1 x_1^{2k+1}$; namely $d_2 = d_1^{\frac{1}{2}} x_1^{k+\frac{1}{2}}$. The proof is completed.

2.5 Comparison of ρ_k , ρ'_k , and ρ''_k

Observe that ρ_k , ρ'_k , and ρ''_k satisfy similar equations. Since $1 < \sqrt{d_1 x_1} < \frac{2}{1 - x_i^{k+1}}$, we have

$$\rho_k'' \le \rho_k' \le \rho_k.$$

For $\lambda \in [\lambda_0, \frac{3}{2}\sqrt{2}]$, x_2 , d_2 , and d_1x_1 are increasing while x_1 is decreasing. Using these facts, it is easy to check that for $k \geq 7$, ρ_k , ρ'_k , and ρ''_k are in the interval $(\lambda_0, \frac{3}{2}\sqrt{2})$.

We have the following lemma.

Lemma 2.13 For $k \geq 7$, we have $\rho_k < \rho''_{k-4}$ and $\rho_k < \rho'_{k-3}$.

Proof Recall that ρ_{k-4}'' is the root of $d_2 = x_1^{k-4}$ and ρ_k is the root of $d_2 = \frac{2x_1^k}{1-x_1^{k+1}}$. We need to show $2 < x_2^4(1-x_1^{k+1})$ for $\lambda \in [\lambda_0, \frac{3}{2}\sqrt{2}]$. For $k \ge 7$, we have

$$\begin{array}{rcl} x_2^4(1-x_1^{k+1}) & \geq & x_2^4-x_1^4 \\ & \geq & (x_2^4-x_1^4)|_{\lambda_0} \\ & > & 2. \end{array}$$

Note that ρ'_{k-3} is the root of $d_2 = \sqrt{d_1x_1}x_1^{k-3}$. It suffices to show $2 < \sqrt{d_1x_1}x_2^3(1-x_1^{k+1})$ for $\lambda \in [\lambda_0, \frac{3}{2}\sqrt{2}]$. We have

$$\sqrt{d_1 x_1} x_2^3 (1 - x_1^{k+1}) \ge \sqrt{d_1 x_1} x_2^3 (1 - x_1^8)
\ge \sqrt{d_1 x_1} x_2^3 (1 - x_1^8)|_{\lambda_0}
> 2.$$

The proof is completed.

3 Proof of Theorem 1.1

The proof of Theorem 1.1 can be naturally divided into two parts. In the first part, we prove that $G_{n,n-e}^{min} \in \mathcal{P}_{n,e}$. In the second part, we prove the other statements in Theorem 1.1.

3.1 Part 1

Let $\rho_{n,n-e}^{min} = \rho(G_{n,n-e}^{min})$ in the rest part of this paper. Now we prove the following theorem, which implies the first part of Theorem 1.1.

Theorem 3.1 If $e \ge 6$ and $n \ge 10e^2 - 74e + 142$, then $G_{n,n-e}^{min} \in \mathcal{P}_{n,e}$.

Proof By Theorem 5.2 of [2] (see page 2), it suffices to show $G_{n,n-e}^{min} \notin \mathcal{P}'_{n,e}$ and $G_{n,n-e}^{min} \notin \mathcal{P}'_{n,e}$. Suppose $G_{n,n-e}^{min} = T'_{(k_1,k_2,\ldots,k_{e-3})} \in \mathcal{P}'_{n,e}$. Note that $T'_{(k_1,k_2,\ldots,k_{e-3})}$ contains sub-trees of type $T'_{(k_1,*)}, T''_{(k_{e-3},*)}$, and $T''_{(*,k_i,*)}$ for $2 \le i \le e-4$. By Lemma 2.4, Lemma 2.11, Corollary 2.2, and Lemma 2.12, we have

$$\begin{array}{lll} \rho_{n,n-e}^{min} & > & \rho_{k_1}', \\ \rho_{n,n-e}^{min} & > & \rho_{2k_{e-3}+3}'', \\ \rho_{n,n-e}^{min} & > & \rho_{k_i}'', & \text{for } 2 \leq i \leq e-4. \end{array}$$

Next, we show that at least one of $k_1, k_2, \ldots, k_{e-3}$ is small. Let $l_1 = \lceil \frac{n-3e+5}{e-3.5} \rceil$. We claim

$$k_1 \le l_1 + 1$$
 or $k_{e-3} \le \frac{l_1 - 3}{2}$ or $\exists i \in \{2, 3, \dots, e - 4\} \ s.t. \ k_i \le l_1.$

Otherwise, we have

$$k_1 \ge l_1 + 2$$
 and $k_{e-3} \ge \frac{l_1 - 2}{2}$ and $k_2, ..., k_{e-4} \ge l_1 + 1$.

We get

$$n = \sum_{i=1}^{e-3} k_i + 2e \ge l_1 + 2 + \frac{l_1 - 2}{2} + (l_1 + 1)(e - 5) + 2e = (e - 3.5)l_1 + 3e - 4 \ge n + 1.$$

Contradiction!

If $k_1 \leq l_1 + 1$, then we have $\rho_{n,n-e}^{min} > \rho'_{l_1+1} > \rho_{l_1+4}$; if $k_{e-3} \leq \frac{l_1-3}{2}$, then we have $\rho_{n,n-e}^{min} > \rho''_{2k_{e-3}+3} > \rho''_{l_1} > \rho_{l_1+4}$; if $k_i \leq l_1$ for some $i \in \{2, \ldots, e-4\}$, then we have $\rho_{n,n-e}^{min} > \rho''_{k_i} \geq \rho''_{l_1} > \rho_{l_1+4}$. In all cases, we have

$$\rho_{n,n-e}^{min} > \rho_{l_1+4}.$$

Let $k = \lfloor \frac{n-2e+2}{e-4} \rfloor$. There exists a tree $T \in \mathcal{P}_{n,e}$, which can be obtained by subdividing some edges on internal paths of $T_{(k-1,k,\ldots,k,k-1)}$. Since $n \geq 10e^2 - 74e + 142$, we have

$$l_1 + 4 = \left\lceil \frac{n - 3e + 5}{e - 3.5} \right\rceil + 4 \le \left\lfloor \frac{n - 2e + 2}{e - 4} \right\rfloor = k.$$

We get

$$\rho_{n,n-e}^{min} > \rho_{l_1+4} \ge \rho(T_{(k-1,k,\dots,k,k-1)}) \ge \rho(T).$$

Contradiction!

Now we assume $G_{n,n-e}^{min}=T_{(k_1,k_2,\dots,k_{e-2})}''\in\mathcal{P}_{n,e}''$. This is very similar to previous case. We must have

$$k_1 \le \frac{l_2 - 3}{2}$$
 or $k_{e-2} \le \frac{l_2 - 3}{2}$ or $\exists i \in \{2, \dots, e - 3\} \ s.t. \ k_i \le l_2$,

where $l_2 = \lceil \frac{n-3e+7}{e-3} \rceil$. A similar argument shows $\rho_{n,n-e}^{min} > \rho_{l_2+4}$. Here we omit the detail. Let $k = \lfloor \frac{n-2e+2}{e-4} \rfloor$. There exists a tree $T \in \mathcal{P}_{n,e}$, which can be obtained by subdividing some edges on internal paths of $T_{(k-1,k,\dots,k,k-1)}$. Since $e \ge 5$ and $n \ge 10e^2 - 74e + 142$, we have $n > 5e^2 - 31e + 50$; thus,

$$l_2 + 4 = \left\lceil \frac{n - 3e + 7}{e - 3} \right\rceil + 4 \le \left\lceil \frac{n - 2e + 2}{e - 4} \right\rceil = k.$$

We get

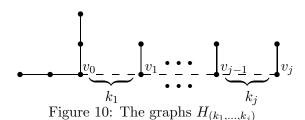
$$\rho_{n,n-e}^{min} > \rho_{l_2+4} \ge \rho(T_{(k-1,k,\dots,k,k-1)}) \ge \rho(T).$$

Contradiction!

Remark 3: Assume $G_{n,n-e}^{min} = T_{(k_1,\dots,k_r)} \in P_{n,e}$. Let $\bar{k} = \frac{\sum_{i=1}^r k_i}{r}$. By Lemma 2.13, we can get $k_i \geq \lfloor \overline{k} + \frac{2}{r} \rfloor - 3$ for $2 \leq i \leq r-1$ and $k_i \geq \lfloor \overline{k} + \frac{2}{r} \rfloor - 2$ for i=1,r whenever $n \geq 9e-30$.

3.2Part 2

From now on, we only consider a tree $T_{(k_1,k_2,...,k_r)}$ in $\mathcal{P}_{n,e}$. (Here r=e-4 through the remaining of the paper.) Let $v_0, v_1, ..., v_r$ be the list (from left to right) of all degree 3 vertices in $T_{(k_1,k_2,\ldots,k_r)} \in \mathcal{P}_{n,e}$. Let $H_{(k_1,k_2,\ldots,k_j)}$ be the graph shown in Figure 10.



Now we define two families of sub-trees of $T_{(k_1,k_2,...,k_r)}$. For i=1,...,r-1, let $L_i=H_{(k_1,k_2,...,k_i)}$ (from the left direction). For j = 2, ..., r, let $R_j = H_{(k_r, k_{r-1}, ..., k_j)}$ (from the right direction). We also define $L_0 = P_5$ and $R_{r+1} = P_5$.

Lemma 3.1 For any $\lambda \geq \rho(T_{(k_1,k_2,...,k_r)})$, we have

1.
$$p_{(L_i,v_i)}(\lambda) \ge 0$$
 and $q_{(L_i,v_i)}(\lambda) \ge 0$ for $i = 0, 1, 2, \dots, r-1$;

2.
$$p_{(R_i,v_{i-1})}(\lambda) \geq 0$$
 and $q_{(R_i,v_{i-1})}(\lambda) \geq 0$ for $j = 2, \ldots, r+1$.

Proof For simplicity, we also write $p_i = p_{(L_i,v_i)}$, $q_i = q_{(L_i,v_i)}$ for i = 0, 1, 2, ..., r - 1, and $p'_j = p_{(R_j,v_{j-1})}$, $q'_j = q_{(R_j,v_{j-1})}$ for j = 2, ..., r + 1. From equation (10), we have $p'_{r+1} = p_0 = 1$ $p_{(P_5,v_0)} = \frac{d_1x_1(\lambda^2-1)}{x_2-x_1} > 0 \text{ and } q'_{r+1} = q_0 = q_{(P_5,v_0)} = \frac{d_2x_2(\lambda^2-1)}{x_2-x_1} > 0 \text{ for any } \lambda > \lambda_0.$ It remains to consider p_i , q_i for $i = 1, 2, \dots, r-1$, and p'_j , q'_j for $j = 2, \dots, r$. Let μ be the

least number such that these functions $p_i(\lambda)$, $q_i(\lambda)$ $p'_j(\lambda)$, $q'_j(\lambda)$ take non-negative values for all $\lambda \geq \mu$.

We need to show such μ exists. By Lemma 2.5, we have $\lim_{\lambda \to +\infty} q_i(\lambda) = +\infty$ and $\lim_{\lambda \to +\infty} q'_j(\lambda) = +\infty$. Since $\lim_{\lambda \to +\infty} p_0 = \lim_{\lambda \to +\infty} \frac{d_1 x_1(\lambda^2 - 1)}{x_2 - x_1} = +\infty$ and $p_i = \frac{1}{x_2 - x_1} (d_1 x_1^{k_i} p_{i-1} + x_2^{k_i - 1} q_{i-1})$ (see Lemma 2.6), by induction on i, we have $\lim_{\lambda \to +\infty} p_i(\lambda) = +\infty$. Similarly, we have $\lim_{\lambda \to +\infty} p'_j(\lambda) = +\infty$. Thus μ is well-defined.

If $\mu \leq \rho(T_{(k_1,k_2,\ldots,k_r)})$, then we are done. Otherwise, we assume $\mu > \rho(T_{(k_1,k_2,\ldots,k_r)})$. Note that μ is always a root of one of those $p_i(\lambda)$, $q_i(\lambda)$, $p_j'(\lambda)$, $q_j'(\lambda)$.

Case (1) There exists an i $(1 \le i \le r - 1)$ such that $p_i(\mu) = 0$. Since $p_i = \frac{1}{x_2 - x_1} (d_1 x_1^{k_i} p_{i-1} + x_2^{k_i - 1} q_{i-1})$, we must have $p_{i-1}(\mu) = q_{i-1}(\mu) = 0$. By Lemma 2.7, we have

$$\phi_{T_{(k_1,k_2,\dots,k_r)}}(\mu) = (x_2 - x_1)(x_2^{k_i - 1}q_{i-1}q'_{i+1} - x_1^{k_i - 1}p_{i-1}p'_{i+1}) \mid_{\mu} = 0.$$

It contradicts to the assumption $\mu > \rho(T_{(k_1,k_2,...,k_r)})$.

Case (2) There exists a j $(2 \le j \le r)$ such that $p'_{j}(\mu) = 0$. This case is symmetric to Case (1).

Case (3) There exists an i $(1 \le i \le r - 1)$ such that $q_i(\mu) = 0$. By Lemma 2.7, we have

$$\phi_{T_{(k_1,k_2,\dots,k_r)}}(\mu) = (x_2 - x_1)(x_2^{k_{i+1}-1}q_iq'_{i+2} - x_1^{k_{i+1}-1}p_ip'_{i+2}) \mid_{\mu} \le 0.$$

It contradicts to $\mu > \rho(T_{(k_1,k_2,...,k_r)})$.

Case (4) There exists a j $(2 \le j \le r)$ such that $q'_i(\mu) = 0$. This case is symmetric to Case (3).

The proof of this Lemma is finished.

The following Lemma gives the lower bound for the spectral radius of a general tree $T_{(k_1,k_2,\dots,k_r)} \in \mathcal{P}_{n,e}$.

Lemma 3.2 Let $\overline{k} = \frac{\sum_{i=1}^{r} k_i}{r}$. We have

$$d_2 \ge \frac{2x_1^{\overline{k} + \frac{2}{r}}}{1 - x_1^{\overline{k} + \frac{2}{r} + 1}}$$

for all $\lambda \ge \rho(T_{(k_1,k_2,...,k_r)})$, where the equality holds if and only if $k_1+1 = k_2 = \cdots = k_{r-1} = k_r+1$ and $\lambda = \rho(T_{(k_1,k_2,...,k_r)})$.

Proof For i = 0, 1, 2, ..., r - 1, we define $t_i = q_i/p_i$. Similarly, for j = 2, ..., r + 1, we define $t'_j = q'_j/p'_j$. For any s > 0, we define

$$f_s(t) = \frac{d_2 x_2^{2s} t - x_2}{x_2^{2s-1} t + d_1} = \frac{d_2 x_2 t - x_1^{2s-2}}{t + d_1 x_1^{2s-1}}, \quad t > 0.$$

We consider the fixed point of $f_s(t)$, which satisfies

$$t^2 - (d_2x_2 - d_1x_1^{2s-1})t + x_1^{2s-2} = 0.$$

This quadratic equation has a unique root x_1^{s-1} when

$$d_2 = 2x_1^s + d_1 x_1^{2s}. (14)$$

We choose $s = s(\lambda)$ to be the root of Equation (14). The line y = t is tangent to the curve $y = f_s(t)$ at $t = x_1^{s-1}$. Because $f_s(t)$ is an increasing and concave function of t, we have

$$f_s(t) \le t, \quad \forall t > 0.$$

For i = 1, ..., r, we have

$$f_{k_i}(t) = f_s(x_2^{2(k_i - s)}t) \le x_2^{2(k_i - s)}t.$$
(15)

By Lemma 2.7, we get

$$\phi_{T_{(k_1,k_2,\ldots,k_r)}} = (x_2 - x_1)(x_2^{k_r - 1}q_{r-1}q'_{r+1} - x_1^{k_r - 1}p_{r-1}p'_{r+1}).$$

Since $\phi_{T_{(k_1,k_2,...,k_r)}} \ge 0$ for all $\lambda \ge \rho(T_{(k_1,k_2,...,k_r)})$, we get

$$t_{r-1}t'_{r+1}x_2^{2(k_r-1)} \ge 1.$$

Note $t'_{r+1} = t_0 = \frac{d_2 x_2}{d_1 x_1} = \frac{d_2}{d_1} x_2^2$. Applying inequality (15) recursively, we have

$$1 \leq \frac{d_2}{d_1} x_2^2 \cdot x_2^{2(k_r - 1)} \frac{q_{r-1}}{p_{r-1}}$$

$$= \frac{d_2}{d_1} x_2^{2k_r} f_{k_{r-1}} (f_{k_{r-2}} (... (f_{k_1} (t_0)...)))$$

$$\leq \frac{d_2}{d_1} x_2^{2k_r} x_2^{2(k_{r-1} - s)} x_2^{2(k_{r-2} - s)} ... x_2^{2(k_1 - s)} t_0$$

$$= \frac{d_2}{d_1} x_2^{2k_r} x_2^{2(k_{r-1} - s)} x_2^{2(k_{r-2} - s)} ... x_2^{2(k_1 - s)} \frac{d_2}{d_1} x_2^2$$

$$= \frac{d_2^2}{d_1^2} x_2^{2(r\overline{k} - (r-1)s + 1)} .$$

We get $d_2 \ge d_1 x_1^{r\overline{k}-(r-1)s+1}$; and the equality holds if and only if $k_1+1=k_2=\cdots=k_{r-1}=k_r+1=s$ and $\lambda=\rho(T_{(k_1,k_2,\ldots,k_r)})$. By Remark 1, $d_2 \ge d_1 x_1^{r\overline{k}-(r-1)s+1}$ is equivalent to

$$d_2 \ge 2x_1^{r\overline{k} - (r-1)s + 2} + d_1 x_1^{2(r\overline{k} - (r-1)s + 2)}. (16)$$

Comparing this inequality with equation (14), we must have $s \leq r\overline{k} - (r-1)s + 2$. Solving s, we get $s \leq \overline{k} + \frac{2}{r}$. Thus,

$$d_2 = 2x_1^s + d_1 x_1^{2s} \ge 2x_1^{\overline{k} + \frac{2}{r}} + d_1 x_1^{2(\overline{k} + \frac{2}{r})}.$$

Applying Remark 1 one more time, we get

$$d_2 \ge \frac{2x_1^{\overline{k} + \frac{2}{r}}}{1 - x_1^{\overline{k} + \frac{2}{r} + 1}}.$$

The proof is completed.

Lemma 3.3 Let $G_{n,n-e}^{min} = T_{(k_1,k_2,...,k_r)}$ and $\overline{k} = \frac{\sum_{i=1}^r k_i}{r}$. Then

$$d_2 \le \frac{2x_1^{\lfloor \overline{k} + \frac{2}{r} \rfloor}}{1 - x_1^{\lfloor \overline{k} + \frac{2}{r} \rfloor + 1}}$$

holds at $\lambda = \rho_{n,n-e}^{min}$.

Proof Let $s = \overline{k} + \frac{2}{r}$. Observe that we can always subdivide some edges on internal paths of $T_{(\lfloor s \rfloor - 1, \lfloor s \rfloor, \ldots, \lfloor s \rfloor, \lfloor s \rfloor - 1)}$ to get a tree T on n vertices and diameter n - e. By Lemma 2.4, we have

$$\rho_{n,n-e}^{min} \le \rho(T) \le \rho(T_{(|s|-1,|s|,\dots,|s|,|s|-1)}) = \rho_{|s|}.$$

By Lemma 2.10, $\rho_{\lfloor s \rfloor}$ is the root of

$$d_2 = \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}}.$$

Since $d_2(\lambda)$ is increasing while $\frac{2x_1^{\lfloor s\rfloor}}{1-x_1^{\lfloor s\rfloor+1}}$ is decreasing on $(\sqrt{2+\sqrt{5}},\infty)$, we get

$$d_2(\rho_{n,n-e}^{min}) \le d_2(\rho_{\lfloor s \rfloor}) = \left. \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}} \right|_{\rho_{\lfloor s \rfloor}} \le \left. \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}} \right|_{\rho_{n,n-e}^{min}}.$$

The proof is completed.

We get the following corollary.

Corollary 3.1 Let $G_{n,n-e}^{min} = T_{(k_1,k_2,...,k_r)} \in \mathcal{P}_{n,e}$ and $s = \frac{1}{r} \sum_{i=1}^r k_i + \frac{2}{r} = \frac{n-2e+2}{e-4}$. We have

$$\frac{2x_1^s}{1 - x_1^{s+1}} \le d_2 \le \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}}$$

holds at $\lambda = \rho(G_{n,n-e}^{min})$. In particular, $\rho(G_{n,n-e}^{min}) = \sqrt{2 + \sqrt{5}} + O\left(\left(\frac{\sqrt{5}-1}{2}\right)^{s/2}\right)$.

Lemma 3.4 Assume $G_{n,n-e}^{min} = T_{(k_1,\dots,k_i,k_{i+1},\dots,k_r)}$ and $\overline{c} = \frac{\rho_{n,n-e}^{min} + \sqrt{(\rho_{n,n-e}^{min})^2 + 4d_1d_2}}{2}}{2}$. Then the following equalities hold at the point $\lambda = \rho_{n,n-e}^{min}$.

$$\overline{c}x_1^{k_i+1} \le d_2 \le \overline{c}x_1^{k_i-1} \quad \text{for } i = 2, ..., r-1;$$
 (17)

$$\sqrt{\overline{c}d_1}x_1^{k_i+1} \le d_2 \le \sqrt{\overline{c}d_1}x_1^{k_i} \quad \text{for } i = 1, r.$$

$$\tag{18}$$

Proof We reuse notations L_i, p_i, q_i, t_i (for i = 0, 1, ..., r-1) and R_j, p'_j, q'_j, t'_j (for j = 2, ..., r+1), which are introduced in Lemma 3.1 and Lemma 3.2.

Choosing any $i \in \{1, ..., r-1\}$, by Lemma 2.7 we have

$$t_i t'_{i+2} x_2^{2(k_{i+1}-1)} = 1$$

at $\lambda = \rho_{n,n-e}^{min}$. This means

$$\frac{d_2 x_2 t_{i-1} - x_1^{2(k_i - 1)}}{t_{i-1} + d_1 x_1^{2k_i - 1}} t'_{i+2} x_2^{2(k_{i+1} - 1)} = 1.$$

We can rewrite it as

$$\left(t_{i-1} - \frac{x_1^{2k_i - 1}}{d_2}\right) \left(t'_{i+2} - \frac{x_1^{2k_{i+1} - 1}}{d_2}\right) = \frac{d_1 d_2 + 1}{d_2^2} x_1^{2(k_i + k_{i+1} - 1)}.$$
(19)

Note $t_i = f_{k_i}(t_{i-1}) = \frac{d_2 x_2 t_{i-1} - x_1^{2(k_i - 1)}}{t_{i-1} + d_1 x_1^{2k_i - 1}} > 0$. We have

$$t_{i-1} > \frac{x_1^{2k_i - 1}}{d_2}. (20)$$

For i = 1, ..., r-1, we apply Lemma 2.9 to $G_1 = T_{(k_1,...,k_i,k_{i+1},...,k_r)}$ and $G_2 = T_{(k_1,...,k_i+1,k_{i+1}-1,...,k_r)}$, where both trees contain a common induced subtree $T_{(k_1,...,k_i+k_{i+1}+1,...,k_r)}$ (after removing one leaf vertex). If $\phi_{G_2}(\rho(G_1)) > 0$, then $\rho(G_1) > \rho(G_2)$. This contradict to the assumption $G_1 = G_{n,n-e}^{\min}.$

We get $\phi_{G_2}(\rho(G_1)) \leq 0$, i.e., $\phi_{T_{(k_1,\dots,k_i+1,k_{i+1}-1,\dots,k_r)}}(\rho_{n,n-e}^{min}) \leq 0$. We apply Lemma 2.8 to obtain the difference of characteristic polynomials of $T_{(k_1,\dots,k_i,k_{i+1},\dots,k_r)}$ and $T_{(k_1,...,k_i+1,k_{i+1}-1,...,k_r)}$,

$$\phi_{T_{(k_1,\ldots,k_i,k_{i+1},\ldots,k_r)}} - \phi_{T_{(k_1,\ldots,k_i+1,k_{i+1}-1,\ldots,k_r)}} = (x_1 - x_2) \left(p_{i-1} q'_{i+2} x_2^{k_{i+1}-k_i-1} - q_{i-1} p'_{i+2} x_1^{k_{i+1}-k_i-1} \right).$$

Evaluating the function above at $\lambda = \rho_{n,n-e}^{min}$, we have

$$(x_1 - x_2) \left(p_{i-1} q'_{i+2} x_2^{k_{i+1} - k_i - 1} - q_{i-1} p'_{i+2} x_1^{k_{i+1} - k_i - 1} \right) \Big|_{\rho_{n,n-e}^{min}} \ge 0.$$

Since $q_{i-1} \ge 0$ and $p'_{i+2} \ge 0$ (from Lemma 3.1), we get $\frac{t'_{i+2}}{t_{i-1}} \le x_1^{2(k_{i+1}-k_i-1)}$ at $\lambda = \rho_{n,n-e}^{min}$. In the rest of the proof, all expressions are evaluated at $\lambda = \rho_{n,n-e}^{min}$. The notation " $|\rho_{n,n-e}^{min}$ " is omitted for simplicity.

On the one hand, by inequality (20), we can substitute $t'_{i+2} \leq t_{i-1} x_1^{2(k_{i+1}-k_i-1)}$ into equation(19) and get

$$\left(t_{i-1} - \frac{x_1^{2k_i - 1}}{d_2}\right) \left(x_1^{2(k_{i+1} - k_i - 1)} t_{i-1} - \frac{x_1^{2k_{i+1} - 1}}{d_2}\right) \ge \frac{d_1 d_2 + 1}{d_2^2} x_1^{2(k_i + k_{i+1} - 1)}.$$

After simplification, we have

$$d_2 t_{i-1}^2 - x_1^{2k_i} \rho_{n,n-e}^{min} t_{i-1} - d_1 x_1^{4k_i} \ge 0.$$

Recall $\bar{c} = \frac{\rho_{n,n-e}^{min} + \sqrt{(\rho_{n,n-e}^{min})^2 + 4d_1d_2}}{2}$. Solving this quadratic inequality, since $t_{i-1} > 0$, we get

$$t_{i-1} \ge \bar{c}x_1^{2k_i}/d_2, \quad i = 1, ..., r-1.$$

By symmetry, we have

$$t'_{i+1} \ge \bar{c}x_1^{2k_i}/d_2, \quad i = 2, ..., r.$$

On the other hand, we substitute $t_{i-1} \ge t'_{i+2} x_2^{2(k_{i+1}-k_i-1)}$ into equation (19). By the similar calculation, we get

$$t'_{i+2} \le \bar{c}x_1^{2(k_{i+1}-1)}/d_2, \quad i = 1, ..., r-1.$$

Changing the index i + 2 to i + 1, we have

$$t'_{i+1} \le \bar{c}x_1^{2(k_i-1)}/d_2, \quad i = 2, ..., r.$$

By symmetry, we have

$$t_{i-1} \le \bar{c}x_1^{2(k_i-1)}/d_2, \quad i = 1, ..., r-1.$$

Combining the inequalities above, we get

$$\frac{\bar{c}}{d_2} x_1^{2k_i} \le t_{i-1} \le \frac{\bar{c}}{d_2} x_1^{2(k_i-1)}, \quad i = 1, ..., r-1, \tag{21}$$

$$\frac{\bar{c}}{d_2} x_1^{2k_i} \le t'_{i+1} \le \frac{\bar{c}}{d_2} x_1^{2(k_i - 1)}, \quad i = 2, ..., r.$$
(22)

Now we apply Lemma 2.7 and get

$$t_{i-1}t'_{i+1}x_2^{2(k_i-1)} = 1. (23)$$

Taking product of inequalities (21), (22), and then substituting $t_{i-1}t'_{i+1}$ into equation (23). After simplification, wet get inequality (17).

When i = 1 or r, we have

$$\frac{\bar{c}}{d_2}x_1^{2k_i} \le t_0 = t'_{r+1} = \frac{d_2}{d_1}x_2^2 \le \frac{\bar{c}}{d_2}x_1^{2(k_i-1)}.$$

Solving for d_2 , we get inequality (18). The proof of this lemma is completed.

Proof of the second part of theorem 1.1. As in the proof of Lemma 3.4, all expressions in this proof are evaluated at $\lambda = \rho_{n,n-e}^{min}$ and " $|\rho_{n,n-e}^{min}|$ " is omitted for simplicity.

By Lemma 3.4, for $2 \le i \le r - 1$, we have

$$\overline{c}x_1^{k_i+1} \le d_2 \le \overline{c}x_1^{k_i-1}.$$

By the definition of \bar{c} , we get

$$2d_2x_1^{k_i+1} \leq \rho_{n,n-e}^{min} + \sqrt{(\rho_{n,n-e}^{min})^2 + 4d_1d_2} \leq 2d_2x_1^{k_i-1}.$$

After solving d_2 and simplifying, we have

$$\frac{\rho_{n,n-e}^{\min}x_1^{k_i+1} + 2x_1^{2k_i+3}}{1 - x_1^{2(k_i+2)}} \le d_2 \le \frac{\rho_{n,n-e}^{\min}x_1^{k_i-1} + 2x_1^{2k_i-1}}{1 - x_1^{2k_i}}.$$

Since $\rho_{n,n-e}^{min} > 2 > 1 + x_1^2 = \rho_{n,n-e}^{min} x_1$, we observe

$$\frac{2x_1^{k_i+1}}{1-x_1^{k_i+2}} < \frac{\rho_{n,n-e}^{\min} x_1^{k_i+1} + 2x_1^{2k_i+3}}{1-x_1^{2(k_i+2)}}$$

and

$$\frac{\rho_{n,n-e}^{\min} x_1^{k_i-1} + 2x_1^{2k_i-1}}{1 - x_1^{2k_i}} < \frac{2x_1^{k_i-2}}{1 - x_1^{k_i-1}}.$$

We obtain

$$\frac{2x_1^{k_i+1}}{1-x_1^{k_i+2}} < d_2 < \frac{2x_1^{k_i-2}}{1-x_1^{k_i-1}} \quad \text{for } 2 \le i \le r-1.$$
 (24)

From Theorem 3.1, we have

$$\frac{2x_1^s}{1 - x_1^{s+1}} \le d_2 \le \frac{2x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}}.$$
 (25)

Combining inequalities (24) and (25), we get

$$\frac{2x_1^{k_i+1}}{1-x_1^{k_i+2}} < \frac{2x_1^{\lfloor s\rfloor}}{1-x_1^{\lfloor s\rfloor+1}},$$

$$\frac{2x_1^{k_i-2}}{1-x_1^{k_i-1}} > \frac{2x_1^s}{1-x_1^{s+1}}.$$

Thus, $\lfloor s \rfloor - 1 < k_i < s + 2$. So $\lfloor s \rfloor < k_i \le \lceil s \rceil + 1$ where i = 2, ..., r - 1. For j = 1 or r, combining inequalities (18) and (25), we have

$$\frac{\sqrt{\overline{c}d_1}}{2} x_1^{k_j+1} \leq \frac{x_1^{\lfloor s \rfloor}}{1 - x_1^{\lfloor s \rfloor + 1}}, \\ \frac{\sqrt{\overline{c}d_1}}{2} x_1^{k_j} \geq \frac{x_1^s}{1 - x_s^{s+1}}.$$

Note that $d_1 \to 2x_1$ and $\overline{c} \to \lambda_0$ as n approaches infinity. For sufficiently large n, we have $x_2^{0.1} < \frac{\lambda_0}{2} < x_2^{0.2}$. We get

$$x_1^{k_j+1+0.45} \le x_1^{\lfloor s \rfloor}$$
 and $x_1^{k_j+0.4} > x_1^s$

So $|s| - 1 \le k_i \le |s|$ for n large enough.

In conclusion, we get

$$|s| - 1 \le k_i \le |s| \le k_i \le \lceil s \rceil + 1$$

for $2 \le i \le r - 1$ and j = 1, r.

Now we will prove item 2. It suffices to show $k_i - k_j \le 2$, for $2 \le i \le r - 1$ and j = 1, r. Suppose that there exist i, j with $i \in \{2, ..., r - 1\}$ and $j \in \{1, r\}$ so that $k_i \ge k_j + 3$. By Lemma 3.4, we have

$$\sqrt{\overline{c}d_1}x_1^{k_j+1} \le d_2 \le \overline{c}x_1^{k_j+2}$$
.

Since $\lambda x_1^2 = (1+x_1^2)x_1 < 2x_1 \le d_1$ for $\lambda \ge \lambda_0$ and $\overline{c} \to \lambda_0$ as n approaches infinity, we have $\overline{c}x_1^{k_j+2} < \sqrt{\overline{c}d_1}x_1^{k_j+1}$ for n large enough. Contradiction!

Now we will prove item 3. By Lemma 3.4, we have $\overline{c}x_1^{k_j+1} \leq d_2 \leq \overline{c}x_1^{k_i-1}$ for all $2 \leq i, j \leq r-1$. This implies $|k_i - k_j| \leq 2$. It is sufficient to show that there are no i, j with $|k_i - k_j| = 2$. Otherwise, suppose there exist $i, j \in \{2, ..., r-1\}$ such that $k_i = k$ and $k_j = k+2$. Without loss of generality, we can assume that i < j and in addition i, j are mostly close to each other. Namely, $k_l = k+1$ for all integer l between i and j.

Applying inequality (17) to $k_i = k$ and $k_j = k + 2$, we have

$$d_2 \geq \overline{c}x_1^{k_i+1} = \overline{c}x_1^{k+1},$$

$$d_2 \leq \overline{c}x_1^{k_j-1} = \overline{c}x_1^{k+1}.$$

Two inequalities above force $d_2 = \overline{c}x_1^{k+1}$. These equalities force $t_{i-1} = t'_{i+1} = x_1^{k-1}$, $t_{j-1} = t'_{j+1} = x_1^{k+1}$ by inequalities (21) and (22).

Consider the function $f(t) = \frac{d_2t - x_2}{x_1t + d_1} = f_k(x_1^{2k}t)$ and let $c = \bar{c}/d_2 = x_2^{k+1}$. It is easy to check $f(c) = \frac{1}{c}$. We claim

$$t_l = x_1^{k+1} \quad \text{ for } i \le l \le j-1.$$

For l = i, we have

$$t_i = f_k(t_{i-1}) = f_k(x_1^{k-1}) = f(x_2^{k+1}) = f(c) = \frac{1}{c} = x_1^{k+1}.$$

By induction on l, we have

$$t_l = f_{k+1}(t_{l-1}) = f_{k+1}(x_1^{k+1}) = f(x_2^{k+1}) = f(c) = \frac{1}{c} = x_1^{k+1}.$$

By Lemma 2.7, we have

$$t_{j-2}t_j'x_2^{2k} = 1.$$

Since $t_{j-2} = x_1^{k+1}$, it implies $t'_j = x_1^{k-1}$. However, we also have

$$t'_{i} = f_{k+2}(t'_{i+1}) = f_{k+2}(x_1^{k+1}) = f(x_2^{k+3}) \neq x_1^{k-1}.$$

Contradiction!

If n-6 is divisible by e-4, then $s=\frac{n-6}{e-2}-4$ is an integer. In this case, the only possible sequence (k_1,k_2,\ldots,k_r) satisfying items 1-3 is $(s-1,s,\ldots,s,s-1)$. In particular, we have $G_{n,n-e}^{min} = T_{(s-1,s,\dots,s,s-1)}.$ The proof is completed.

Proofs of Theorems 1.3 and 1.4

e=74.1

Let $G_{n,n-7}^{min} = T_{(k_1,k_2,k_3)} \in \mathcal{P}_{n,7}$. Note $k_1 + k_2 + k_3 = n - 14$. By Theorem 1.1, here are all the possible graphs for $G_{n,n-7}^{min}$.

Case 1.
$$\sum_{i=1}^{3} k_i = 3k$$
. We have $(k_1, k_2, k_3) = (k, k, k)$ or $(k, k+1, k-1)$.

Case 2.
$$\sum_{i=1}^{3} k_i = 3k + 1$$
. We have $(k_1, k_2, k_3) = (k, k + 1, k)$.

Case 3.
$$\sum_{i=1}^{3} k_i = 3k + 2$$
. We have $(k_1, k_2, k_3) = (k, k + 2, k)$ or $(k, k + 1, k + 1)$.

To simplify the proof of Theorem 1.3, we introduce the following short notations. We have

$$\begin{aligned} p_0 &:= p_{(L_0,v_0)} = \frac{\lambda^2 - 1}{x_2 - x_1} d_1 x_1, \\ q_0 &:= q_{(L_0,v_0)} = \frac{\lambda^2 - 1}{x_2 - x_1} d_2 x_2, \\ p^{(k-1)} &:= p_{(H_{(k-1)},v_1)} = \frac{\lambda^2 - 1}{(x_2 - x_1)^2} (d_1^2 x_1^k + d_2 x_2^{k-1}), \\ q^{(k-1)} &:= q_{(H_{(k-1)},v_1)} = \frac{\lambda^2 - 1}{(x_2 - x_1)^2} (d_2^2 x_2^k - d_1 x_1^{k-1}), \\ p^{(k)} &:= p_{(H_{(k)},v_1)} = \frac{\lambda^2 - 1}{(x_2 - x_1)^2} (d_1^2 x_1^{k+1} + d_2 x_2^k), \\ q^{(k)} &:= q_{(H_{(k)},v_1)} = \frac{\lambda^2 - 1}{(x_2 - x_1)^2} (d_2^2 x_2^{k+1} - d_1 x_1^k), \\ p^{(k+1)} &:= p_{(H_{(k+1)},v_1)} = \frac{\lambda^2 - 1}{(x_2 - x_1)^2} (d_1^2 x_1^{k+2} + d_2 x_2^{k+1}), \\ q^{(k+1)} &:= q_{(H_{(k+1)},v_1)} = \frac{\lambda^2 - 1}{(x_2 - x_1)^2} (d_1^2 x_1^{k+2} + d_1 d_2 x_1 + d_2^2 x_2^{2k+1} - d_1), \\ p^{(k,k+1)} &:= p_{(H_{(k,k+1)},v_2)} = \frac{\lambda^2 - 1}{(x_2 - x_1)^3} (d_1^3 x_1^{2k+2} + d_1 d_2 x_2 - d_1^2 x_1^{2k+1} - d_2). \end{aligned}$$

Proof of Theorem 1.3. We will compare the spectral radius of the possible graphs listed above in three cases separately.

Case 1.
$$\sum_{i=1}^{3} k_i = 3k$$
.

By Lemma 2.8, we have

$$\phi_{T_{(k,k,k)}} - \phi_{T_{(k,k+1,k-1)}} = (x_1 - x_2) \left(p^{(k)} q_0 x_1 - q^{(k)} p_0 x_2 \right)$$

$$= -\frac{(\lambda^2 - 1)^2}{(x_2 - x_1)^2} \left[(d_2 x_1 + 1) d_1^2 x_1^k - (d_1 x_2 - 1) d_2^2 x_2^k \right]$$

$$= \frac{(d_2 x_1 + 1)(\lambda^2 - 1)^2}{(x_2 - x_1)^2} \left(d_2^2 x_2^k - d_1^2 x_1^k \right).$$

In the last step, we applied the fact $d_2x_1 + 1 = d_1x_2 - 1$.

By Lemma 2.10 and Remark 1, $\rho(T_{(k,k+1,k)})$ (= ρ_{k+1}) satisfies $d_2x_2^{k/2} = d_1x_1^{k/2}$. The largest root of $\phi_{T_{(k,k,k)}} - \phi_{T_{(k,k+1,k-1)}} = 0$ is ρ_{k+1} .

Noting that $d_2^2x_2^k-d_1^2x_1^k$ is an increasing function of $\lambda\in\left(\sqrt{2+\sqrt{5}},\frac{3}{2}\sqrt{2}\right)$ for sufficiently large k. By Lemma 2.4, we have $\rho_{k+1}=\rho(T_{(k,k+1,k)})<\rho(T_{(k,k,k)})$. Evaluating $\phi_{T_{(k,k,k)}}-\phi_{T_{(k,k+1,k-1)}}$ at $\lambda=\rho(T_{(k,k,k)})$, we get $\phi_{T_{(k,k+1,k-1)}}(\rho(T_{(k,k,k)}))<0$. Thus, by Lemma 2.2, $\rho(T_{(k,k,k)})<\rho(T_{(k,k+1,k-1)})$ and $G_{n,n-7}^{min}=T_{(k,k,k)}$.

Case 2.
$$\sum_{i=1}^{3} k_i = 3k + 1$$
. We must have $G_{n,n-7}^{min} = T_{(k,k+1,k)}$.

Case 3.
$$\sum_{i=1}^{3} k_i = 3k + 2$$
.

Similarly by Lemma 2.8, we have

$$\phi_{T_{(k,k+1,k+1)}} - \phi_{T_{(k,k+2,k)}} = \frac{(d_2x_1 + 1)(\lambda^2 - 1)^2}{(x_2 - x_1)^2} \left(d_2^2x_2^k - d_1^2x_1^k \right).$$

Noting that $d_2^2 x_2^k - d_1^2 x_1^k$ is an increasing function of $\lambda \in \left(\sqrt{2+\sqrt{5}}, \frac{3}{2}\sqrt{2}\right)$ for sufficiently large k. We have $\phi_{T_{(k,k+1,k+1)}}(\lambda) < \phi_{T_{(k,k+2,k)}}(\lambda)$ for any $\sqrt{2+\sqrt{5}} \le \lambda < \rho_{k+1}$. By Lemma 2.4, we get $\rho(T_{(k,k+1,k+1)}) < \rho(T_{(k,k+1,k)}) = \rho_{k+1}$. Thus, $\phi_{T_{(k,k+1,k+1)}}(\rho(T_{(k,k+2,k)})) < 0$. It follows $\rho(T_{(k,k+1,k+1)}) > \rho(T_{(k,k+2,k)}).$ So $G_{n,n-7}^{min} = T_{(k,k+2,k)}.$

The proof of Theorem 1.3 is completed.

4.2 e=8

Now we let $G_{n,n-8}^{min} = T_{(k_1,k_2,k_3,k_4)} \in \mathcal{P}_{n,8}$. By Theorem 1.1, all the possible graphs for $G_{n,n-8}^{min}$

Case 1. If
$$\sum_{i=1}^{4} k_i = 4k$$
, then $(k_1, k_2, k_3, k_4) = (k, k, k, k)$, $(k, k, k+1, k-1)$, $(k, k+1, k, k-1)$, or $(k-1, k+1, k+1, k-1)$.

Case 2. If
$$\sum_{i=1}^{4} k_i = 4k+1$$
, then $(k_1, k_2, k_3, k_4) = (k, k+1, k, k)$ or $(k, k+1, k+1, k-1)$.

Case 3. If
$$\sum_{i=1}^{4} k_i = 4k + 2$$
, then $(k_1, k_2, k_3, k_4) = (k, k + 1, k + 1, k)$.

Case 4. If
$$\sum_{i=1}^{4} k_i = 4k + 3$$
, then $(k_1, k_2, k_3, k_4) = (k, k + 1, k + 1, k + 1)$ or $(k, k + 1, k + 2, k)$.

Proof of Theorem 1.4. Similarly, we denote $p^{(k,k)} = P_{(H_{(k,k)},v_2)}, q^{(k,k)} = q_{(H_{(k,k)},v_2)}, p^{(k-1,k+1)} = q_{(k,k)}$ $P_{(H_{(k-1,k+1)},v_2)}$, and $q^{(k-1,k+1)} = q_{(H_{(k-1,k+1)},v_2)}$. We will compare the spectral radius of all possible graphs listed in four cases above.

Case 1.
$$\sum_{i=1}^{4} k_i = 4k$$
.

First we prove

$$\rho(T_{(k,k,k,k)}) = \rho(T_{(k,k,k+1,k-1)}) = \rho(T_{(k-1,k+1,k+1,k-1)})$$

By Lemma 2.3, it is easy to see

$$\rho(T_{(k,k,k,k)}) = \rho(T_{(k-1,k)}) = \rho(T_{(k-1,k+1,k+1,k-1)}).$$

Applying Lemma 2.7 to these graphs, we get

$$\begin{split} \phi_{T_{(k,k,k,k)}} &= p^{(k,k)}q^{(k)}x_2^{k-1}(x_2-x_1)\left(\frac{q^{(k,k)}}{p^{(k,k)}}-\frac{p^{(k)}}{q^{(k)}}x_1^{2k-2}\right),\\ \phi_{T_{(k,k,k+1,k-1)}} &= p^{(k,k)}q^{(k-1)}x_2^k(x_2-x_1)\left(\frac{q^{(k,k)}}{p^{(k,k)}}-\frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}\right),\\ \phi_{T_{(k,k,k+1,k-1)}} &= p^{(k-1,k+1)}q^{(k)}x_2^{k-1}(x_2-x_1)\left(\frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}}-\frac{p^{(k)}}{q^{(k)}}x_1^{2k-2}\right),\\ \phi_{T_{(k-1,k+1,k+1,k-1)}} &= p^{(k-1,k+1)}q^{(k-1)}x_2^k(x_2-x_1)\left(\frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}}-\frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}\right). \end{split}$$

Let $\rho = \rho(T_{(k,k,k,k)}) = \rho(T_{(k-1,k+1,k+1,k-1)})$ and $\rho' = \rho(T_{(k,k,k+1,k-1)})$. Write $J(\lambda) = p^{(k,k)}q^{(k-1)}x_2^k(x_2 - x_1)$ and $K(\lambda) = p^{(k-1,k+1)}q^{(k)}x_2^{k-1}(x_2 - x_1)$. By Lemma 3.1, $J(\rho) > 0$ and $K(\rho) > 0$.

Note that ρ is the root of both equations

$$\frac{q^{(k,k)}}{p^{(k,k)}} = \frac{p^{(k)}}{q^{(k)}} x_1^{2k-2} \quad \text{and} \quad \frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}} = \frac{p^{(k-1)}}{q^{(k-1)}} x_1^{2k}. \tag{26}$$

Note that ρ' is the root of both equations

$$\frac{q^{(k,k)}}{p^{(k,k)}} = \frac{p^{(k-1)}}{q^{(k-1)}} x_1^{2k} \quad \text{and} \quad \frac{q^{(k-1,k+1)}}{p^{(k-1,k+1)}} = \frac{p^{(k)}}{q^{(k)}} x_1^{2k-2}. \tag{27}$$

We have

$$\phi_{T_{(k,k,k+1,k-1)}}(\rho) = J(\rho) \left(\frac{p^{(k)}}{q^{(k)}} x_1^{2k-2} - \frac{p^{(k-1)}}{q^{(k-1)}} x_1^{2k} \right) \Big|_{\rho}$$

$$= K(\rho) \left(\frac{p^{(k-1)}}{q^{(k-1)}} x_1^{2k} - \frac{p^{(k)}}{q^{(k)}} x_1^{2k-2} \right) \Big|_{\rho}.$$

Thus, $\phi_{T_{(k,k,k+1,k-1)}}(\rho)^2 = -J(\rho)K(\rho)\left(x_1^{2k-2}\frac{p^{(k)}}{q^{(k)}} - \frac{p^{(k-1)}}{q^{(k-1)}}x_1^{2k}\right)^2\Big|_{\rho} \le 0$. We get $\phi_{T_{(k,k,k+1,k-1)}}(\rho) = -\frac{1}{2}\int_{0}^{\infty} dt dt dt$ 0. Similarly, we can prove $\phi_{T_{(k,k,k,k)}}(\rho') = 0$. Hence, we get $\rho = \rho'$. Now we prove $\rho(T_{(k,k,k+1,k-1)}) < \rho(T_{(k,k+1,k,k-1)})$. By Lemma 2.8, we have

$$\phi_{T_{(k,k,k+1,k-1)}} - \phi_{T_{(k,k+1,k,k-1)}} = (x_1 - x_2) \left(p^{(k)} q^{(k-1)} - q^{(k)} p^{(k-1)} \right) = d_1 d_2 \lambda^2 (\lambda^2 - 1)^2 > 0$$

for any $\lambda > \lambda_0$. So $\rho(T_{(k,k,k+1,k-1)}) < \rho(T_{(k,k+1,k,k-1)})$. We are done in this case.

Case 2. $\sum_{i=1}^{4} k_i = 4k + 1$.

Similarly, by Lemma 2.8, we have

$$\phi_{T_{(k,k+1,k,k)}} - \phi_{T_{(k,k+1,k+1,k-1)}} = (x_1 - x_2) \left(p^{(k,k+1)} q_0 - q^{(k,k+1)} p_0 \right)$$

$$= \frac{(d_2 x_1 + 1)(\lambda^2 - 1)^2 x_2^{2k+1}}{(x_2 - x_1)^3} \left(d_2^3 - 2d_1 d_2 x_1^{2k+1} - d_1^3 x_1^{4k+2} \right).$$

Here we use proof by contradiction. Suppose $G_{n,n-8}^{min}=T_{(k,k+1,k+1,k-1)}$. By Lemma 3.4, $d_2 = \sqrt{\overline{c}d_1}x_1^k$ at $\lambda = \rho(T_{(k,k+1,k+1,k-1)})$. Note $\overline{c} \to \lambda_0$ as $n \to \infty$. When n is large enough, we will get $\overline{c} > (2 + \epsilon)x_1$ for some constant $\epsilon > 0$. Thus, we get

$$d_2^2 = \overline{c}d_1x_1^{2k} > (2+\epsilon)d_1x_1^{2k+1}.$$

For n large enough, we have $\phi_{T_{(k,k+1,k,k)}} - \phi_{T_{(k,k+1,k+1,k-1)}} > 0$ at $\lambda = \rho(T_{(k,k+1,k+1,k-1)})$. Equivalently $\phi_{T_{(k,k+1,k,k)}}(\rho(T_{(k,k+1,k+1,k-1)})) > 0$. By Lemma 2.9, we get $\rho(T_{k,k+1,k,k}) < \rho(T_{k,k+1,k+1,k-1})$. Contradiction! Hence, we have $G_{n,n-8}^{min} = T_{k,k+1,k,k}$.

Case 3. $\sum_{i=1}^{\infty} k_i = 4k + 2$. There is only one possible graph $T_{(k,k+1,k+1,k)}$.

Case 4.
$$\sum_{i=1}^{4} k_i = 4k + 3$$
.

Similarly by Lemma 2.8, we have

$$\begin{split} &\phi_{T_{(k,k+1,k+1,k+1)}} - \phi_{T_{(k,k+1,k+2,k)}} \\ &= (x_1 - x_2) \left(p^{(k,k+1)} q_0 - q^{(k,k+1)} p_0 \right) \\ &= \frac{(d_2 x_1 + 1) (\lambda^2 - 1)^2 x_2^{2k+1}}{(x_2 - x_1)^3} \left(d_2^3 - 2 d_1 d_2 x_1^{2k+1} - d_1^3 x_1^{4k+2} \right) \\ &< \frac{(d_2 x_1 + 1) (\lambda^2 - 1)^2 x_2^{2k+1}}{(x_2 - x_1)^3} \left(d_2^3 - 2 d_1 d_2 x_1^{2k+1} \right) \\ &= \frac{d_2 (d_2 x_1 + 1) (\lambda^2 - 1)^2 x_2^{2k+1}}{(x_2 - x_1)^3} \left(d_2^2 - 2 d_1 x_1^{2k+1} \right). \end{split}$$

We now suppose $G_{n,n-8}^{min}=T_{(k,k+1,k+1,k+1)}$ in this case. By Lemma 3.4, $d_2=\sqrt{\overline{c}d_1}x_1^{k+1}$ at $\lambda=\rho(T_{(k,k+1,k+1,k+1)})$. Recall that $\overline{c}\to\lambda_0$ as $n\to\infty$. When n is large enough, we get $\overline{c}<2x_2$. Thus $d_2=\sqrt{\overline{c}d_1}x_1^{k+1}<\sqrt{2d_1x_2}x_1^{k+1}$. We get $\phi_{T_{(k,k+1,k+2,k)}}(\rho(T_{(k,k+1,k+1,k+1)}))>0$. Applying Lemma 2.9 with $G_2=T_{(k,k+1,k+2,k)}$ and $G_1=T_{(k,k+1,k+1,k+1)}$, we have $\rho(T_{k,k+1,k+2,k})<\rho(T_{k,k+1,k+1,k+1})$. Contradiction! Hence $G_{n,n-8}^{min}=T_{k,k+1,k+2,k}$. The proof is completed.

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